

Densest geodesic ball packings to $S^2 \times \mathbf{R}$ space groups generated by screw motions ^{*}

B. Schultz, J. Szirmai[†]

Budapest University of Technology and
Economics Institute of Mathematics,
Department of Geometry

July 7, 2014

Abstract

In this paper we study the locally optimal geodesic ball packings with equal balls to the $S^2 \times \mathbf{R}$ space groups having rotation point groups and their generators are screw motions. We determine and visualize the densest simply transitive geodesic ball arrangements for the above space groups, moreover we compute their optimal densities and radii. The densest packing is derived from the $S^2 \times \mathbf{R}$ space group **3qe. I. 3** with packing density ≈ 0.7278 .

E. Molnár has shown in [9], that the Thurston geometries have an unified interpretation in the real projective 3-sphere \mathcal{PS}^3 . In our work we shall use this projective model of $S^2 \times \mathbf{R}$ geometry.

1 Introduction

The packing of spheres has been studied by mathematicians for centuries. Finding the densest packing of balls in the Euclidean space is called the Kepler-problem or conjecture, which was solved by Thomas Hales, who proved, with the use of computers, that Keplers original guess was correct [6].

^{*}AMS Classification 2000: 52C17, 52C22, 53A35, 51M20

[†]E-mail: schultzb@math.bme.hu, szirmai@math.bme.hu

In the 3-dimensional hyperbolic \mathbf{H}^3 and spherical space \mathbf{S}^3 the problem of the ball packing was widely investigated in a lot of papers (e.g. [2]), but there are several open questions in this topic for example related to the horoball and hyperball packings in \mathbf{H}^3 (see [7], [19], [22]).

In [23] the second author has extended the problem of finding the densest geodesic and translation ball (or sphere) packing for the other 3-dimensional homogeneous geometries (Thurston geometries) $\mathbf{S}^2 \times \mathbf{R}$, $\mathbf{H}^2 \times \mathbf{R}$, $\widetilde{\mathbf{SL}_2 \mathbf{R}}$, Nil, Sol, [15], [16], [18], [20], [21].

In this paper we consider the $\mathbf{S}^2 \times \mathbf{R}$ geometry which can be derived by the direct product of the spherical plane \mathbf{S}^2 and the real line \mathbf{R} . In [3] J. Z. Farkas has classified and given the complete list of the space groups in $\mathbf{S}^2 \times \mathbf{R}$. The $\mathbf{S}^2 \times \mathbf{R}$ manifolds up to similarity and diffeomorphism were classified by E. Molnár and J. Z. Farkas in [4]. In [17] the geodesic balls and their volumes were studied, moreover, we have introduced the notion of the geodesic ball packing and its density and determined the densest simply and multiply transitive geodesic ball packings for generalized Coxeter space groups of $\mathbf{S}^2 \times \mathbf{R}$, respectively. Among these groups the density of the densest packing is ≈ 0.8245 .

In [18] we have studied the simply transitive locally optimal ball packings to the $\mathbf{S}^2 \times \mathbf{R}$ space groups having Coxeter point groups and at least one of the generators is a non-trivial glide reflection. We have determined the densest simply transitive geodesic ball arrangements for the above space groups. Moreover, their optimal densities and radii were determined. The density of the densest packing of the above space groups is ≈ 0.8041 .

Moreover, a candidate of the densest geodesic ball packing is described in [23]. In the Thurston geometries the greatest known density was ≈ 0.8533 that is not realized by a packing with *equal balls* of the hyperbolic space \mathbf{H}^3 . However, that is attained, e.g., by a *horoball packing* of $\overline{\mathbf{H}}^3$ where the ideal centres of horoballs lie on the absolute figure of $\overline{\mathbf{H}}^3$ inducing the regular ideal simplex tiling $(3, 3, 6)$ by its Coxeter-Schläfli symbol. In [23] we have presented a geodesic ball packing in the $\mathbf{S}^2 \times \mathbf{R}$ geometry whose density is ≈ 0.8776 .

In this paper we study the locally optimal ball packings to the $\mathbf{S}^2 \times \mathbf{R}$ space groups belonging to the *screw motion groups*, i.e., the generators \mathbf{g}_i ($i = 1, 2, \dots, m$) of its point group Γ_0 are rotations, and either any translation parts are zero or at least one of the possible translation parts of the above generators differs from zero (see [18]). We determine and visualize the densest simply transitive geodesic ball arrangements for the above space groups, moreover we compute their optimal densities and radii.

2 The structure of the $S^2 \times \mathbf{R}$ geometry

Now, we shall discuss the simply transitive ball packings to a given space group. But let us start first with the necessary concepts.

$S^2 \times \mathbf{R}$ geometry can be derived by the direct product of the spherical plane S^2 and the real line \mathbf{R} . The points in $S^2 \times \mathbf{R}$ geometry are described by (P, p) where $P \in S^2$ and $p \in \mathbf{R}$.

The isometry group $Isom(S^2 \times \mathbf{R})$ of $S^2 \times \mathbf{R}$ can be derived by the direct product of the isometry group of the spherical plane $Isom(S^2)$ and the isometry group of the real line $Isom(\mathbf{R})$. The structure of an isometry group $\Gamma \subset Isom(S^2 \times \mathbf{R})$ is the following: $\Gamma := \{(A_1 \times \rho_1), \dots, (A_n \times \rho_n)\}$, where $A_i \times \rho_i := A_i \times (R_i, r_i) := (g_i, r_i)$, $i \in \{1, 2, \dots, n\}$, and $A_i \in Isom(S^2)$, R_i is either the identity map $1_{\mathbf{R}}$ of \mathbf{R} or the point reflection $\bar{1}_{\mathbf{R}}$. $g_i := A_i \times R_i$ is called the linear part of the transformation $(A_i \times \rho_i)$ and r_i is its translation part.

The multiplication formula is the following:

$$(A_1 \times R_1, r_1) \circ (A_2 \times R_2, r_2) = ((A_1 A_2 \times R_1 R_2, r_1 R_2 + r_2). \quad (2.1)$$

A group of isometries $\Gamma \subset Isom(S^2 \times \mathbf{R})$ is called *space group* if the linear parts form a finite group Γ_0 called the point group of Γ . Moreover, the translation parts to the identity of this point group are required to form a one dimensional lattice L_Γ of \mathbf{R} . It can be proved that the space group Γ exactly described above has a compact fundamental domain \mathcal{F}_Γ . We characterize the spherical plane groups by the *Macbeath-signature* (see [8], [24]).

*In this paper we deal with a class of the $S^2 \times \mathbf{R}$ space groups **1q. I. 1; 1q. I. 2; 3q. I. 1; 3q. I. 2; 3qe. I. 3; 8. I. 1; 8. I. 2; 9. I. 1; 9. I. 2; 10. I. 1**; (with a natural parameter $q \geq 2$, see [3]) where each of them belongs to the screw motion groups.*

2.1 Geodesic curves and balls in $S^2 \times \mathbf{R}$ space

In [17] and [18] we have described the equation system of the geodesic curve and so the geodesic sphere:

$$\begin{aligned} x(\tau) &= e^{\tau \sin v} \cos(\tau \cos v), \quad y(\tau) = e^{\tau \sin v} \sin(\tau \cos v) \cos u, \\ z(\tau) &= e^{\tau \sin v} \sin(\tau \cos v) \sin u, \quad -\pi < u \leq \pi, \quad -\frac{\pi}{2} \leq v \leq \frac{\pi}{2} \end{aligned} \quad (2.2)$$

with radius $\rho = \tau \geq 0$ and centre $x(0) = 1$, $y(0) = 0$, $z(0) = 0$, and longitude u , altitude v , as geographical coordinates.

In [17] we have proved that a geodesic sphere $S(\rho)$ in $\mathbf{S}^2 \times \mathbf{R}$ space is a simply connected surface in \mathbf{E}^3 if and only if $\rho \in [0, \pi)$. Namely, if $\rho \geq \pi$ then there is at least one $v \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ so that $y(\tau, v) = z(\tau, v) = 0$, i.e., selfintersection would occur. Thus we obtain the following

Proposition 2.1 *The geodesic sphere and ball with radius ρ exists in the $\mathbf{S}^2 \times \mathbf{R}$ space if and only if $\rho \in [0, \pi)$.*

We have obtained (see [17]) the volume formula of the geodesic ball $B(\rho)$ of radius ρ by the metric tensor g_{ij} , by the Jacobian of (2.2) and a careful numerical Maple computation for given ρ by the following integral:

Theorem 2.2

$$\begin{aligned} \text{Vol}(B(\rho)) &= \int_V \frac{1}{(x^2 + y^2 + z^2)^{3/2}} dx dy dz = \\ &= \int_0^\rho \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \int_{-\pi}^\pi |\tau \cdot \sin(\cos(v)\tau)| du dv d\tau = 2\pi \int_0^\rho \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} |\tau \cdot \sin(\cos(v)\tau)| dv d\tau. \end{aligned} \quad (2.3)$$

2.2 On fundamental domains

A type of the fundamental domain of a studied space group can be combined as a fundamental domain of the corresponding spherical group with a part of a real line segment. This domain is called $\mathbf{S}^2 \times \mathbf{R}$ prism (see [17]). *This notion will be important to compute the volume of the Dirichlet-Voronoi cell of a given space group because their volumes are equal and the volume of a $\mathbf{S}^2 \times \mathbf{R}$ prism can be calculated by Theorem 2.3.* The p -gonal faces of a prism called cover-faces, and the other faces are the side-faces. The midpoints of the side edges form a "spherical plane" denoted by Π . It can be assumed that the plane Π is the base plane in our coordinate system (see (2.2)) i.e. the fibre coordinate $t = 0$.

From [17] we recall

Theorem 2.3 *The volume of a $\mathbf{S}^2 \times \mathbf{R}$ trigonal prism $\mathcal{P}_{B_0 B_1 B_2 C_0 C_1 C_2}$ and of a digonal prism $\mathcal{P}_{B_0 B_1 C_0 C_1}$ in $\mathbf{S}^2 \times \mathbf{R}$ (see Fig. 1.a-b) can be computed by the following formula:*

$$\text{Vol}(\mathcal{P}) = \text{Vol}(\mathcal{A}) \cdot h \quad (2.4)$$

where $\text{Vol}(\mathcal{A})$ is the area of the spherical triangle $A_0 A_1 A_2$ or digon $A_0 A_1$ in the base plane Π with fibre coordinate $t = 0$, and $h = B_0 C_0$ is the height of the prism.

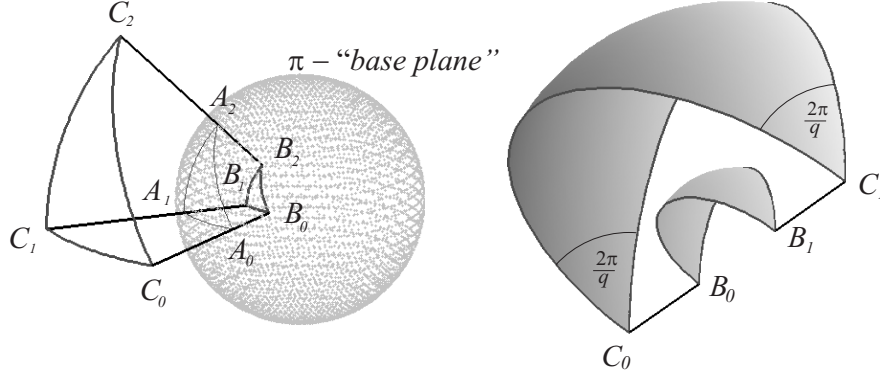


Figure 1: Prism-like fundamental domains

3 Geodesic ball packings under discrete isometry groups

A $S^2 \times \mathbf{R}$ space group Γ has a compact fundamental domain. Usually the shape of the fundamental domain of a group of S^2 is not determined uniquely but the area of the domain is finite and unique by its combinatorial measure. Thus the shape of the fundamental domain of a crystallographic group of $S^2 \times \mathbf{R}$ is not unique, as well.

In the following let Γ be a fixed by *screw motions generated* space group of $S^2 \times \mathbf{R}$. We will denote by $d(X, Y)$ the distance of two points X, Y by definition (2.2).

Definition 3.1 We say that the point set

$$\mathcal{D}(K) = \{X \in S^2 \times \mathbf{R} : d(K, X) \leq d(K^g, X) \text{ for all } g \in \Gamma\}$$

is the Dirichlet–Voronoi cell (*D-V cell*) to Γ around the kernel point $K \in S^2 \times \mathbf{R}$.

Definition 3.2 We say that

$$\Gamma_X = \{g \in \Gamma : X^g = X\}$$

is the stabilizer subgroup of $X \in S^2 \times \mathbf{R}$ in Γ .

Definition 3.3 Assume that the stabilizer $\Gamma_K = \mathbf{I}$ i.e. Γ acts simply transitively on the orbit of a point K . Then let \mathcal{B}_K denote the greatest ball of centre K inside

the D-V cell $\mathcal{D}(K)$, moreover let $\rho(K)$ denote the radius of \mathcal{B}_K . It is easy to see that

$$\rho(K) = \min_{\mathbf{g} \in \Gamma \setminus \mathbf{I}} \frac{1}{2} d(K, K^{\mathbf{g}}).$$

The Γ -images of \mathcal{B}_K form a ball packing \mathcal{B}_K^Γ with centre points K^Γ .

Definition 3.4 The density of ball packing \mathcal{B}_K^Γ is

$$\delta(K) = \frac{\text{Vol}(\mathcal{B}_K)}{\text{Vol}\mathcal{D}(K)}.$$

It is clear that the orbit K^Γ and the ball packing \mathcal{B}_K^Γ have the same symmetry group, moreover this group contains the starting crystallographic group Γ :

$$\text{Sym}K^\Gamma = \text{Sym}\mathcal{B}_K^\Gamma \geq \Gamma.$$

Definition 3.5 We say that the orbit K^Γ and the ball packing \mathcal{B}_K^Γ is *characteristic* if $\text{Sym}K^\Gamma = \Gamma$, else the orbit is not characteristic.

3.1 Simply transitive ball packings

Our problem is to find a point $K \in \mathbf{S}^2 \times \mathbf{R}$ and the orbit K^Γ for Γ such that $\Gamma_K = \mathbf{I}$ and the density $\delta(K)$ of the corresponding ball packing $\mathcal{B}^\Gamma(K)$ is maximal. In this case the ball packing $\mathcal{B}^\Gamma(K)$ is said to be *optimal*.

The lattice of Γ has a free parameter $p(\Gamma)$. Then we have to find the densest ball packing on K for fixed $p(\Gamma)$, and vary p to get the optimal ball packing.

$$\delta^{opt}(\Gamma) = \max_{K, p(\Gamma)} (\delta(K)) \quad (3.1)$$

Let Γ be a fixed by *screw motions generated* group. The stabiliser of K is trivial i.e. we are looking the optimal kernel point in a 3-dimensional region, inside of a fundamental domain of Γ with free fibre parameter $p(\Gamma)$. It can be assumed by the homogeneity of $\mathbf{S}^2 \times \mathbf{R}$, that the fibre coordinate of the center of the optimal ball is zero.

3.2 Optimal ball packings to space groups **1q. I.**

We consider those by screw motions generated groups in $\mathbf{S}^2 \times \mathbf{R}$ whose point groups Γ_0 determine spherical groups, characterized by their Macbeath signature. The first set among them is **1q. I.** which contain two space groups **1q. I. 1**, **1q. I. 2**:

$$(+, 0, [q, q], \{\}) \times 1_{\mathbf{R}}, \quad q \geq 1, \quad q \in \mathbf{N}$$

$$\Gamma_0 = (g_1 | g_1^q = 1),$$

where q is an integer parameter, which shows the degree of the rotation generating the point group. It is easy to see that to the parameters $q = 1$, $q = 2$ do not exist ball packings thus we assume, that $3 \leq q \in \mathbf{N}$. The possible translation parts of the generators of Γ_0 will be determined by the defining relations of the point group. Finally, from the so-called Frobenius congruence relations we obtain two classes of non equivariant solutions:

$$\tau \cong 0, \text{ or } \frac{k}{q}, \quad k := 1 \dots \left\lfloor \frac{q}{2} \right\rfloor \quad (\text{i.e. lower integer part of } \frac{q}{2}).$$

If $\tau \cong 0$ then we get the $\mathbf{S}^2 \times \mathbf{R}$ space group **1q. I. 1** and if $\tau \cong \frac{k}{q}$, $k := 1 \dots \left\lfloor \frac{q}{2} \right\rfloor$ then we get the $\mathbf{S}^2 \times \mathbf{R}$ space group **1q. I. 2**.

We note here, that iff the greatest common divisor $(k, q) = 1$, then the group $\Gamma = \mathbf{1q. I. 2}$ will be fixed point free and the factor space $\mathbf{S}^2 \times \mathbf{R} / \Gamma$ will be a compact orientable manifold (space form).

The fundamental domains of their point groups are spherical digons $B_0 B_1$ with angles $\frac{2\pi}{q}$ lying in the base plane Π (see Fig. 1).

We shall apply the Cartesian homogeneous coordinate system introduced in Section 2.

3.2.1 Optimal ball packing to space group **1q. I. 1**

We can assume, that g_1 is a rotation about the z -axis through angle $\frac{2\pi}{q}$ ($q \geq 3$). The translation part in the corresponding $\mathbf{S}^2 \times \mathbf{R}$ space group is zero. Therefore, the group contain an arbitrary fibre translation τ . The fundamental domain ($D - V$ cell) of such a space group is a $\mathbf{S}^2 \times \mathbf{R}$ prism with height $h = |\tau|$ whose volume can be calculated by the Theorem 2.3.

It can be assumed by the homogeneity of $\mathbf{S}^2 \times \mathbf{R}$, that the fibre coordinate of the center of the optimal ball is zero and it is clear, that the centre of the optimal ball is coincide with the centre of the digon $B_0 C_0 B_1 C_1$ (see Fig. 1). Therefore, the radius

of the incircle or insphere of the optimal ball is $R^{opt} = \frac{\pi}{q}$. Moreover, we obtain the locally densest ball arrangement if the height of the prism is $h_q^{opt} = 2R_q^{opt} = \frac{2\pi}{q}$. These, locally densest ball arrangements, depending on q are denoted by \mathcal{B}_q^{opt} .

Theorem 3.6 *The ball arrangement \mathcal{B}_3^{opt} provides the optimal ball packing to the $\mathbb{S}^2 \times \mathbb{R}$ space group $1q. I. 1$ with density $\delta^{opt}(1q. I. 1) \approx 0.50946$.*

Proof

The fundamental domain of their point groups are a spherical digon $\mathcal{A}_q = B_0B_1$ with angles $\frac{2\pi}{q}$ lying in the base plane Π (see Fig. 1). The area of the a digon is $Vol(\mathcal{A}_q) = \frac{4\pi}{q}$, while the radius of the incircle or insphere is $R^{opt} = \frac{\pi}{q}$. The volume of the locally optimal $D - V$ cell \mathcal{P}_q (prism-like domain) of the ball arrangement \mathcal{B}_q is $Vol(\mathcal{P}_q) = \frac{4\pi^2}{q^2}$ (see Theorem 2.3). The volume $Vol(B_q^{opt})$ of the corresponding optimal ball B_q^{opt} of radius $R^{opt} = \frac{\pi}{q}$ can be computed by the Theorem 2.2 and thus we obtain the densities δ_q^{opt} of the ball packings \mathcal{B}_q^{opt} for arbitrary given parameter $3 \leq q \in \mathbb{N}$. Moreover, if the parameter q is sufficiently large then the volume of the optimal ball $Vol(B_q^{opt})$ is approximately equal to the Euclidean one which is direct proportion to $\frac{1}{q^3}$. Therefore, $\delta^{opt}(1q. I. 1)$ is a strictly decrease function of q and thus, \mathcal{B}_3^{opt} provides the densest ball arrangement. \square

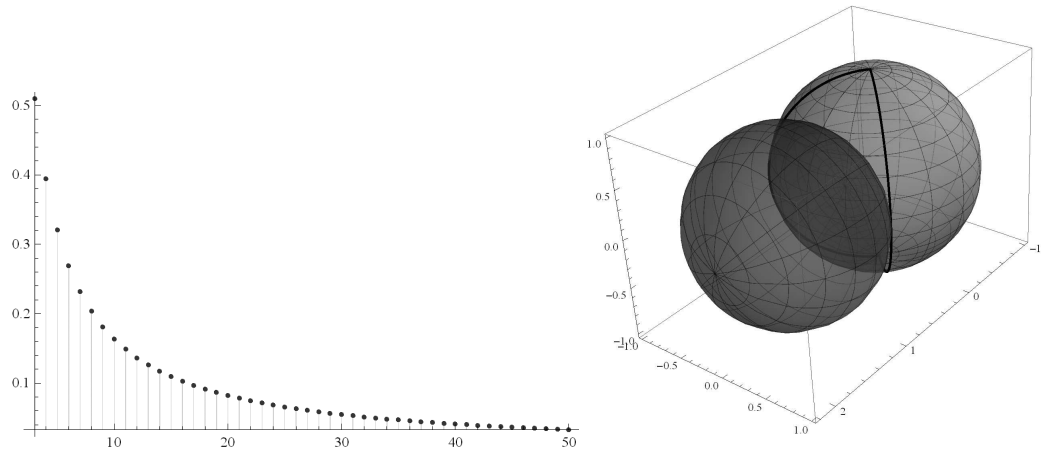


Figure 2: The optimal densities of group $1q. I. 1$ for parameters $q = 3, 4, 5, 6, \dots$ and the optimal ball with the base plane Π if $q = 4$

3.3 Optimal ball packing to space groups 8. I.

We consider those screw motions generated groups **8. I. 1** and **8. I. 2** (using the Macbeath signature $(+, 0, [2, 3, 3], \{\}) \times 1_{\mathbf{R}}$) whose point group Γ_0 is determined by the spherical group

$$\Gamma_0 = (g_1, g_2 | g_1^2 = g_2^3 = (g_1 g_2)^3 = 1).$$

where g_1, g_2 are two rotations with degrees of 2 and 3 respectively. Fig. 3 shows a spherical fundamental domain $A_1 A_2 A_3 A_4 A_5$ of this group that is a spherical pentagon lying in the base plane Π . It is a spherical Dirichlet-Voronoi domain $\mathcal{D}(K)$ with kernel point K . Moreover let F be the midpoint of the spherical segment $A_1 A_2$. Here g_1 is the 2-rotation about the fibre line f_F through the point F , g_2 is the 3-rotation about the fibre line f_{A_3} through the point A_3 and $g_1 g_2$ is the 3-rotation about the fibre line f_{A_5} , as well.

The possible translation parts of the generators will be determined by the defining relations of the point group. From the Frobenius congruence relations we can obtain two classes of non-equivariant solutions: $(\tau_1, \tau_2) \cong (0, 0)$, or $(0, \frac{1}{3})$ and so two space groups **8. I. 1** and **8. I. 2** (see [3]).

3.3.1 Optimal ball packing to space group 8. I. 1

First let us consider the space group $\Gamma_1 = \mathbf{8. I. 1}$, where the translation parts of the generators are $(\tau_1, \tau_2) = (0, 0)$. In this case the group is only generated by two rotations g_1, g_2 and the group contains a nonzero radial translation τ . The fundamental domain of the space group Γ_1 is a pentagonal prism $\mathcal{P}(K) = B_1 B_2 B_3 B_4 B_5 C_1 C_2 C_3 C_4 C_5$ which is derived from the spherical fundamental domain $\mathcal{D}(K) = A_1 A_2 A_3 A_4 A_5$ by translations $\tau/2$ and $-\tau/2$ (see Fig. 3). $\mathcal{P}(K)$ is also a $D - V$ cell of the considered group with kernel point K , as well. Let $\mathcal{B}(R)$ denote a geodesic ball packing of $\mathbf{S}^2 \times \mathbf{R}$ space with balls $B(R)$ of radius R where their centres give rise to the orbit K^{Γ_1} . In the following we consider to each ball packing the *possible smallest translation part* $\tau(K, R)$ (see Fig. 3) depending on Γ_1 , K and R . A fundamental domain of Γ is its prism-like $D - V$ cell $\mathcal{P}(K)$ around the kernel point K . It is clear that the optimal ball \mathcal{B}_K has to touch some faces of its $D - V$ cell. The volume of $\mathcal{P}(K)$ can be calculated by the area of the spherical fundamental domain $\mathcal{D}(K)$ and by the height $\tau(R, K)$. The images of $\mathcal{D}(K)$ form a congruent prism tiling by the discrete isometry group Γ . For the density of the packing it is sufficient to relate the volume of the optimal ball to that of the solid $\mathcal{P}(K)$ (see Definition 3.4). It is clear, that it is sufficient to study

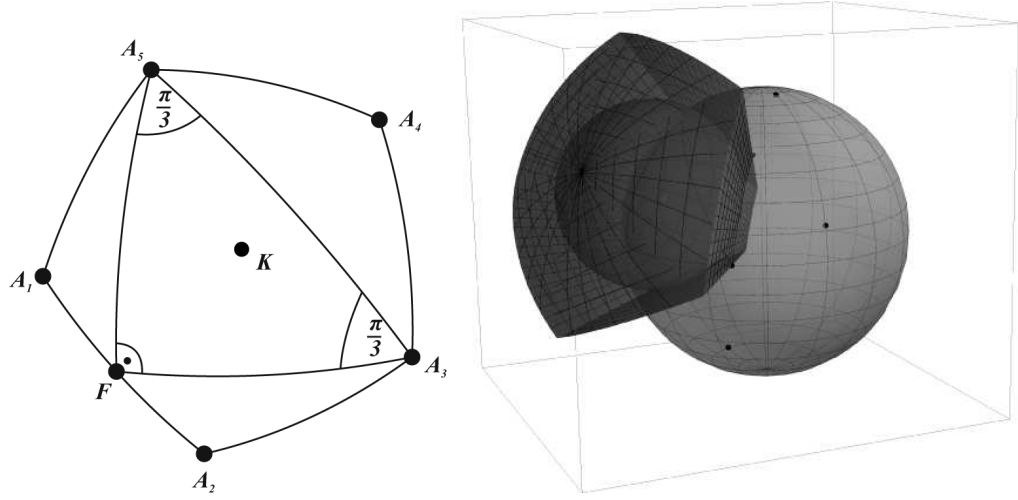


Figure 3: The fundamental domain of the point group of the space group 8. I. 1 and the optimal 5-gonal prism-like $D - V$ -cell $\mathcal{P}(K^{opt})$ with the base plane

the kernel point as the point of the spherical triangle (lying in the base plane Π) FA_3A_5 with angles $\frac{\pi}{3}, \frac{\pi}{2}, \frac{\pi}{3}$ without its vertices.

We shall apply the Cartesian homogeneous coordinate system introduced in Section 2.

Theorem 3.7 *The coordinates of the kernel point K^{opt} , the radius and the density of the optimal ball packings $\mathcal{B}^{opt}(R)$ of the $S^2 \times \mathbb{R}$ space group 8. I. 1 are*

$$K^{opt} = \left(\sqrt{\frac{5+\sqrt{5}}{10}}, \frac{1}{2}\sqrt{\frac{\sqrt{5}-1}{\sqrt{5}}}, \frac{1}{2}\sqrt{\frac{\sqrt{5}-1}{\sqrt{5}}} \right), \quad R^{opt} = \arccos \sqrt{\frac{5+\sqrt{5}}{10}}.$$

$$\delta^{opt}(\mathbf{8. I. 1}) = \frac{Vol(\mathcal{B}(R^{opt}))}{Vol(\mathcal{P}(K^{opt}))} \approx 0.6005$$

Proof

Our goal is to find the optimal kernel point K^{opt} lying in the spherical triangle FA_3A_5 , $K \notin \{F, A_3, A_5\}$ of the optimal Dirichlet-Voronoi cell $\mathcal{P}(K^{opt})$ and the optimal sphere radius R^{opt} , so that the density $\delta(K)$ of the ball packing is maximal. We can assume that g_1 is the 2-rotation about the x axis, while the axis of 3-rotation g_2 is in the $[x, y]$ plane.

Because the translation parts of the generators g_i ($i = 1, 2$) in the corresponding $S^2 \times \mathbb{R}$ space group are zero, therefore in this case the balls have a spherical

shell-like arrangement $\mathcal{D}(K) = A_1 A_2 A_3 A_4 A_5$ and the group contains a fibre translation τ .

The optimal ball arrangement $\mathcal{B}^{opt}(R^{opt})$ has to satisfy the following requirements:

1. $\frac{\sqrt{3}}{2}d(K, K^{g_2}) = d(K, K^{g_1})$
2. $2R^{opt} = d(K, K^{g_1}) = d(K, K^\tau)$

The first condition ensures the touching of the optimal sphere with the side neighbouring spheres of the prism \mathcal{P} on the level of the base sphere, while the third condition requires the touching of the optimal sphere and its radial translated images. By solving the above system of equations, we get the center K^{opt} of the insphere

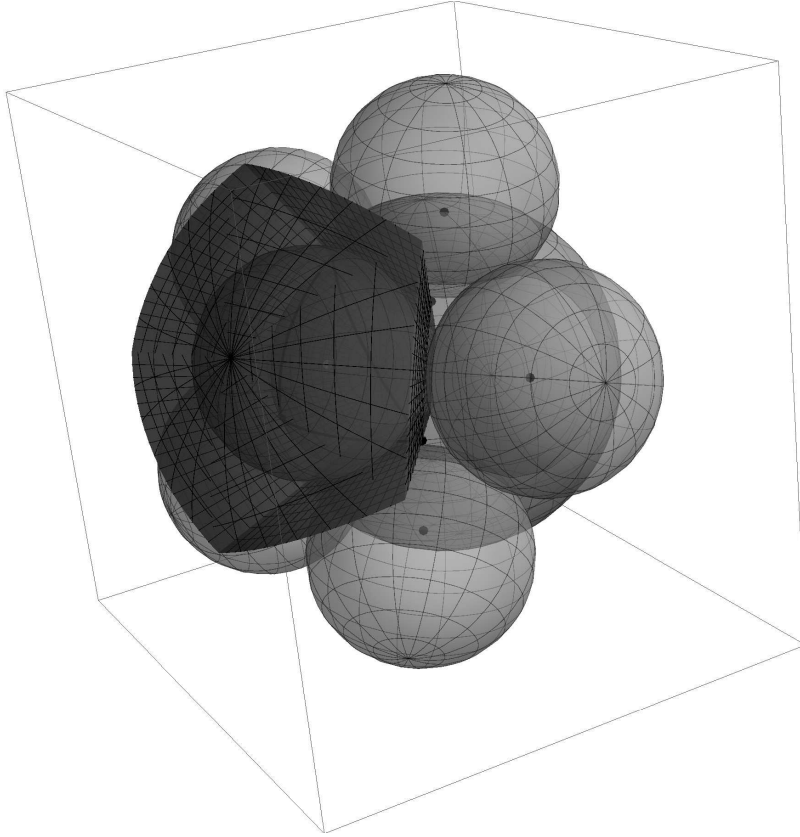


Figure 4: The optimal ball arrangement $\mathcal{B}^{opt}(R^{opt})$ with a optimal prism-like $D - V$ cell $\mathcal{P}(K^{opt})$ of space group 8. I. 1.

$$K^{opt} = \left(\sqrt{\frac{5+\sqrt{5}}{10}}, \frac{1}{2}\sqrt{\frac{\sqrt{5}-1}{\sqrt{5}}}, \frac{1}{2}\sqrt{\frac{\sqrt{5}-1}{\sqrt{5}}} \right), \text{ and its radius } R^{opt} = \arccos \sqrt{\frac{5+\sqrt{5}}{10}}.$$

It is easy to see, that the area of the base polygon $Vol(\mathcal{P}(K^{opt})) = 2 \cdot Vol(FA_3A_5\Delta) = \frac{\pi}{3}$, so the volume of the Dirichlet-Voronoi cell can be computed by the Theorem 2.3. Moreover, we get by Theorem 2.2 the volume of the insphere $Vol(B(R^{opt})) \approx 0.6962$ and thus using the density formula given in Definition 3.4 we obtain the optimal density $\delta^{opt}(8. I. 1) \approx 0.6005$ (see Fig. 4). \square

3.3.2 Optimal ball packing to space group 8. I. 2

We get the space group $\Gamma_2 = 8. I. 2$ if the translation part of the generators are $(\tau_1, \tau_2) = (0, \frac{1}{3})$ i.e. $\tau_1 = \tau$; $\tau_2 = \frac{\tau}{3}$.

Similarly to the above case the spherical fundamental domain of its point group is a spherical pentagon $\mathcal{D}(K) = A_1A_2A_3A_4A_5$ lying in the base plane Π (see Fig. 2. a). It can be assumed by the homogeneity of $\mathbf{S}^2 \times \mathbf{R}$, that the fibre coordinate of the center of the optimal ball is zero and it lies in the spherical triangle FA_3A_5 , $K \notin \{F, A_3, A_5\}$ using the above denotations.

We shall apply for the computations the Cartesian homogeneous coordinate system introduced in Section 2.

We consider an arbitrary point $K(x^0, x^1, x^2, x^3)$ of spherical triangle FA_3A_5 , $K \notin \{F, A_3, A_5\}$ in the above coordinate system in our model.

Let $\mathcal{B}(R)$ denote a geodesic ball packing of $\mathbf{S}^2 \times \mathbf{R}$ space with balls $B(R)$ of radius R where their centres give rise to the orbit K^{Γ_2} . In the following we consider to each ball packing *the possible smallest translation part* $\tau(K, R)$ depending on Γ_2 , K and R . A fundamental domain of Γ_2 is its $D - V$ cell $\mathcal{P}(K)$ with kernel point K which is not a prism. The optimal ball has to touch some faces of its $D - V$ cell so that *the balls of the packing form a locally stable arrangement*.

The volume of $\mathcal{P}(K)$ is equal to the volume of the prism which is given by the fundamental domain of the point group Γ_0 of Γ and by the height $|\tau(R, K)|$. The images of $\mathcal{P}(K)$ by our discrete isometry group Γ_2 covers the $\mathbf{S}^2 \times \mathbf{R}$ space without overlap. For the density of the packing it is sufficient to relate the volume of the optimal ball to that of the solid $\mathcal{P}(K)$ (see Definition 3.4). It is clear, that the densest ball arrangement $\mathcal{B}_{\Gamma_2}^{opt}(R)$ of balls $B(R)$ has to hold the following requirements:

$$1. \ d(K, K^{g_1}) = 2R = d(K, K^{g_2\tau_2}) = d(K, K^{g_1g_2\tau_2})$$

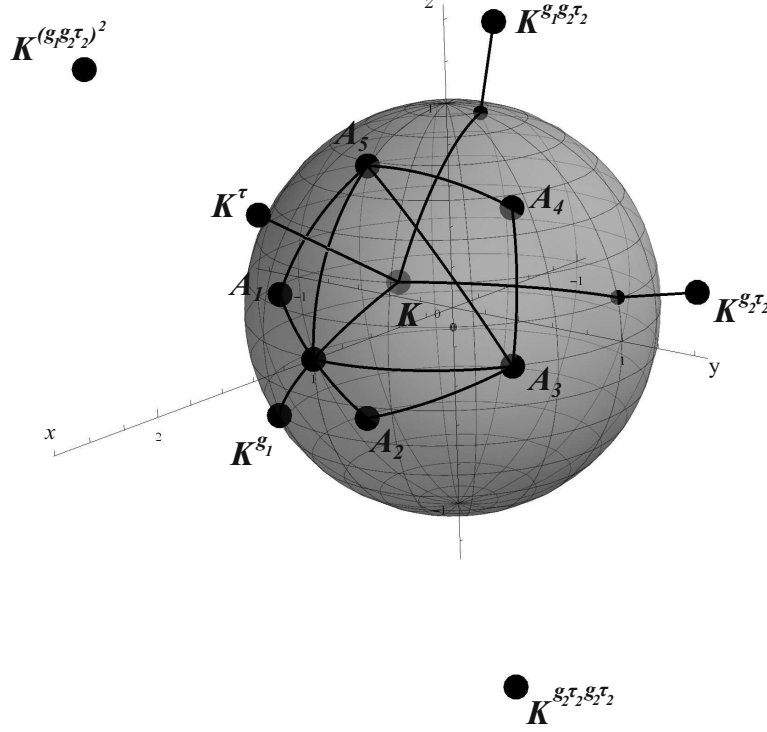


Figure 5: A part of the orbit K^{Γ_2} where $K(x^0, x^1, x^2, x^3) \in FA_3A_5$, $K \notin \{F, A_3, A_5\}$.

$$2. \ d(K, K^\tau) \geq 2R$$

$$3. \ d(K^{g_2g_2\tau_2\tau_2}, K^{g_1g_2g_1g_2\tau_2\tau_2}) \geq 2R,$$

where d is the distance function of $S^2 \times \mathbb{R}$ space.

The ball packings described by the requirements above form a one parameter class of ball arrangements by the parameter τ . We can now examine the density function $\delta(\tau)$ and find its maximum.

We consider two main ball arrangements:

- a. We denote by $\mathcal{B}_{\Gamma_2}^a(R_a, K_a)$ the packing, where the above requirements and

$d(K, K^\tau) = 2R$ hold. (This is the case, where the kissing number Ω of the balls is maximal $\Omega = 7$.)

- b. We denote by $\mathcal{B}_{\Gamma_2}^b(R_b, K_b)$ the packing, where the above requirements and $d(K^{g_2g_2\tau_2}, K^{g_1g_2g_1g_2\tau_2\tau_2}) = 2R$ hold. (This is the case, where the radius R of the spheres is maximal, here $\Omega = 5$)

Theorem 3.8 *The ball packing $\mathcal{B}_{\Gamma_2}^a(R_a, K_a)$ provides the optimal ball packing to the $S^2 \times \mathbf{R}$ space group 8. I. 2 with density $\delta^{opt}(8. I. 2) \approx 0.6587$.*

Proof

The corresponding τ values to the ball arrangements $\mathcal{B}_{\Gamma_2}^a(R_a, K_a)$ and $\mathcal{B}_{\Gamma_2}^b(R_b, K_b)$ are $\tau_a \approx 1.1608$ and $\tau_b \approx 3.5071$. It is easy to see, that for any $\tau < \tau_a$ then $\delta(\tau) < \delta(\tau_a) \approx 0.6587$, and we get also that if $\tau = \tau_b$ then the radius of the sphere is maximal, so for $\tau > \tau_b$ the density must be smaller than $\delta(\tau_b) \approx 0.5289$.

The derivatives of the density function $\delta(\tau) = \frac{Vol(B(\tau))}{Vol(\mathcal{P}(K^\tau))}$ can be approximated by numerical methods to an arbitrary precision. Careful approximation and investigation of the first and second derivatives of the density function shows, that the second derivative is strictly positive on the interval $[\tau_a, \tau_b]$, therefore the maximum of the density function must be in one of the endpoints of the interval.

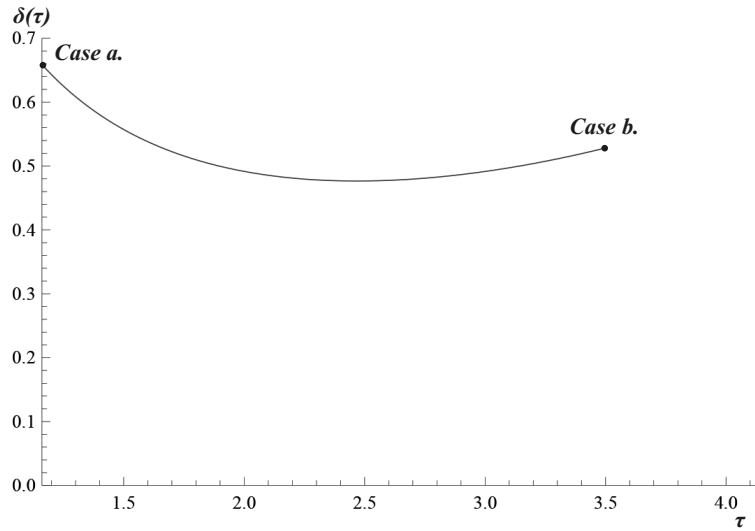
First we determine the coordinates of the points K_i , the radii R_i ($i = a, b$) of the balls, the volumes of the corresponding balls and the densities in both cases. Finally we get the following solutions, where the computations were carried out by *Wolfram Mathematica 8*:

$$\begin{aligned} R_a &= 0.5804, K_a = (0.8362, 0.3877, 0.3877), \delta(\tau_a) \approx 0.6587, \\ R_b &= 0.7847, K_b = (0.7075, 0.4996, 0.4996), \delta(\tau_b) \approx 0.5289, \end{aligned}$$

Therefore, the ball packing $\mathcal{B}_{\Gamma_2}^a(R_a, K_a)$ provides the maximal density to the $S^2 \times \mathbf{R}$ space group 8. I. 2. \square

The remaining groups 1q. I. 2, 3q. I. 1, 3qe. I. 2, 3qe. I. 3, 9. I. 1, 9. I. 2, 10. I. 1 can be studied with the same way, as we have described previously. Finally we have summarized our results in the following Table. Finally we get the following

Theorem 3.9 *The densest geodesic ball packings to $S^2 \times \mathbf{R}$ space groups generated by screw motions is derived by the space group 3qe. I. 3 with maximal packing density $\delta^{opt}(3qe. I. 3) \approx 0.7278$.*

Figure 6: The density function $\delta(\tau)$ of group **8. I. 2.**

Group	(τ_1, τ_2)	Optimal radius	Optimal density
1q. I. 1	(0)	$R = \frac{\pi}{3}$	$\delta \approx 0.5094$ (with $q = 3$)
1q. I. 2	$(\frac{k}{q})$	$R \approx 1.1107$	$\delta \approx 0.5678$ (with $q = 3, k = 1$)
3q. I. 1	$(0, 0)$	$R = \frac{\pi}{4}$	$\delta \approx 0.5919$ (with $q = 3$)
3q. I. 2	$(\frac{1}{2}, \frac{1}{2})$	$R \approx 0.8417$	$\delta \approx 0.6758$
3qe. I. 3	$(0, \frac{1}{2})$	$R \approx 0.8752$	$\delta \approx 0.7278$
8. I. 1	$(0, 0)$	$R = \arccos \sqrt{\frac{5+\sqrt{5}}{10}}$	$\delta \approx 0.6004$
8. I. 2	$(0, \frac{1}{3})$	$R \approx 0.5804$	$\delta \approx 0.6587$
9. I. 1	$(0, 0)$	$R \approx 0.3812$	$\delta \approx 0.5758$
9. I. 2	$(\frac{1}{2}, 0)$	$R \approx 0.4189$	$\delta \approx 0.6937$
10. I. 1	$(0, 0)$	$R \approx 0.2341$	$\delta \approx 0.5458$

References

- [1] Böröczky, K. Packing of spheres in spaces of constant curvature, *Acta Math. Acad. Sci. Hungar.*, (1978) **32** , 243–261.
- [2] Böröczky, K. – Florian, A. Über die dichteste Kugelpackung im hyperbolischen Raum, *Acta Math. Acad. Sci. Hungar.*, (1964) **15** , 237–245.

- [3] Farkas, Z. J. The classification of $S^2 \times \mathbb{R}$ space groups, *Beitr. Algebra Geom.*, **42**(2001), 235–250.
- [4] Farkas, Z. J. – Molnár, E. Similarity and diffeomorphism classification of $S^2 \times \mathbb{R}$ manifolds, *Steps in Diff. Geometry, Proc. of Coll. on Diff. Geom. 25–30 July 2000. Debrecen (Hungary)*, (2001), 105–118,
- [5] Fejes Tóth, L. Reguläre Figuren, *Akadémiai Kiadó*, Budapest, (1965).
- [6] Hales, C. T. "A proof of the Kepler conjecture", *Ann. Math.*, **162/3** (2005), 1065–1185, DOI:10.4007/annals.2005.162.1065.
- [7] Kozma, T. R. – Szirmai, J. Optimally dense packings for fully asymptotic Coxeter tilings by horoballs of different types, *Monatsh. Math.*, **168** (2012), 27–47, DOI: 10.1007/s00605-012-0393-x.
- [8] Macbeath, A. M The classification of non-Euclidean plane crystallographic groups. *Can. J. Math.*, **19** (1967), 1192–1295.
- [9] Molnár, E. The projective interpretation of the eight 3-dimensional homogeneous geometries, *Beitr. Algebra Geom.*, **38** (1997), No. 2, 261–288.
- [10] Molnár, E. – Szirmai, J. On Nil crystallography. *Symmetry: Culture and Science*, **17/1-2** (2006), 55–74.
- [11] Molnár, E. – Szirmai, J. Volumes and geodesic ball packings to the regular prism tilings in $\widetilde{SL_2\mathbb{R}}$ space. *Publ. Math. Debrecen*, **84/1-2**, (2014), 189–203, DOI: 10.5486/PND.2014.5832.
- [12] Pallagi, J. – Schultz, B. – Szirmai, J. Visualization of geodesic curves, spheres and equidistant surfaces in $S^2 \times \mathbb{R}$ space, *KoG*, **14**, (2010), 35–40.
- [15] Szirmai, J. The densest geodesic ball packing by a type of Nil lattices, *Beitr. Algebra Geom.*, **48** No. 2, (2007), 383–398.
- [16] Szirmai, J. The densest translation ball packing by fundamental lattices in Sol space, *Beitr. Algebra Geom.*, **51** No. 2, (2010), 353–373.

- [17] Szirmai, J. Geodesic ball packings in $S^2 \times \mathbb{R}$ space for generalized Coxeter space groups. *Beitr. Algebra Geom.*, **52**, (2011), 413 – 430.
- [18] Szirmai, J. Simply transitive geodesic ball packings to glide reflections generated $S^2 \times \mathbb{R}$ space groups, *Ann. Mat. Pur. Appl.* (2013), DOI: 10.1007/s10231-013-0324-z.
- [19] Szirmai, J. Horoball packings and their densities by generalized simplicial density function in the hyperbolic space, *Acta Math. Hung.*, **136/1-2**, (2012), 39–55, DOI: 10.1007/s10474-012-0205-8.
- [20] Szirmai, J. Lattice-like translation ball packings in Nil space, *Publ. Math. Debrecen*, **80/3-4**, (2012), 427– 440, DOI: 10.5486/PND.2012.5117.
- [21] Szirmai, J. Geodesic ball packings in $H^2 \times \mathbb{R}$ space for generalized Coxeter space groups, *Math. Commun.*, **17/1**, (2012), 151-170.
- [22] Szirmai, J. Horoball packings to the totally asymptotic regular simplex in the hyperbolic n-space, *Aequat. Math.*, **85**, (2013), 471-482, DOI: 10.1007/s00010-012-0158-6.
- [23] Szirmai, J. A candidate for the densest packing with equal balls in Thurston geometries. *Beitr. Algebra Geom.*, (to appear) (2013) DOI: 10.1007/s13366-013-0158-2.
- [24] Thurston, W. P. (and LEVY, S. editor) *Three-Dimensional Geometry and Topology*. Princeton University Press, Princeton, New Jersey, Vol **1** (1997).